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APSIM's Water and Nitrogen Modules and Simulation of the Dynamics of Water and Nitrogen in Fallow Systems

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ABSTRACT

APSIM (Agricultural Production Systems Simulator) is a software system which provides a flexible structure for the simulation of climatic and soil management effects on growth of crops in farming systems and changes in the soil resource. The focus of this paper is the predictive performance of APSIM for simulation of soil water and nitrate nitrogen in contrasting soils (vertisols and alfisols) and environments. The three APSIM modules that determine the dynamics of water, carbon, and nitrogen in the soil system (viz. SOILWAT, SOILN and RESIDUE v.1) are described in terms of the processes represented, with particular emphasis on aspects of their coding that differ from their precursors in CERES and PERFECT. The most fundamental change is in SOILN, which now provides a formal balance of both carbon and nitrogen in the soil and includes a labile soil organic matter pool that decomposes more rapidly than the bulk of the soil organic matter. Model performance, in terms of prediction of soil water and nitrate, is evaluated during fallows, thereby avoiding complications arising from water use and nitrogen uptake by a crop. One data set is from a long-term experiment on a vertisol in southeast Queensland which studied two tillage treatments (conventional and zero tillage) in combination with fertiliser nitrogen inputs for the growth of wheat; soil water and nitrate were measured twice each year (pre-planting and post-harvest). The second comes from experiments at Katherine, Northern Territory, where legume leys growing on alfisols were chemically killed and ensuing changes in soil water and nitrate were measured during a single season. For both datasets, the predictive ability of the model was satisfactory for water and nitrate, in terms *of both the total amounts in the whole profile and their distribution with depth. Since neither of these datasets included measurements of the runoff component of the water balance, this aspect of model performance was evaluated, and shown to be generally good, using data from a third source where runoff had been measured from contour bay catchments.*

INTRODUCTION

Simulation models are valuable tools in the analysis of farming systems, particularly for assessing impacts of climatic variability and the long-term consequences of alternative management strategies. Models are complementary to experimentation which is invariably constrained by the prevailing seasonal conditions, limitations in the treatments imposed, and the duration of the experimentation. They are a means of extrapolation of knowledge, derived from experimentation, to other situations—other seasons, other soils, and different managements such as crop sequences, tillage, and residue management practices. To do this, the simulation package must deal credibly with the season-to-season variability in production and the long-term trends in production in response to changes in the soil resource.

APSIM (Agicultural Production Systems Simulator) is a software system that allows models of crops, pastures, soil water, nutrients, and erosion to be flexibly configured to simulate diverse production systems (McCown *et al.*, 1996). A key feature of APSIM, which distinguishes it from models of single crops, is the central position of the soil rather than the crops. Changes in the status of the soil state variables are simulated continuously in response to weather and management. Crops come and go, finding the soil in a particular state and leaving it in an altered state. Another feature is its modular structure: high order processes (for example, production of a crop, soil water balance, and dynamics of soil nitrogen) are represented as separate modules with 'plug in–pull out' capability. This arrangement offers great flexibility for comparing alternative representations of different parts of the system without modification to the rest of the model.

In describing APSIM and its development, McCown *et al.* (1996) dealt with the priorities of the need to simulate the performance of cropping systems, in terms of both crops and soil, and software requirements. This paper focuses on their third priority, namely predictive performance. Water and nitrogen are frequently the major limitations to crop production which are subject to management control. If a model is to simulate production credibly, it must be able to predict changes in soil water and nitrogen with sufficient accuracy, since these are two factors to which the crop responds.

The paper describes the three APSIM modules, viz. SOILWAT v.1, SOILN v.1, and RESIDUE v.1, that determine the dynamics of water, carbon and nitrogen in the soil system. Their performance in simulating soil water and nitrate nitrogen (N) in fallow systems on contrasting soil types is reported. By restricting the evaluation to fallows, it is possible to assess performance without complications arising from water use and nitrogen uptake by crops. These aspects are better considered as part of the crop growth routines and will be the subject of other reports.

MATERIALS AND METHODS

Model description

Much of the code that constitutes the APSIM SOILWAT, SOILN, and RESIDUE modules has evolved from earlier experience with, firstly, models of the CERES family, notably CERES-Maize (Jones and Kiniry, 1986) and, secondly, PERFECT (Littleboy *et al.*, 1989). PERFECT was developed primarily to simulate the effects of erosion on the productivity of vertisols in the Australian subtropics but it did not deal with nitrogen. PERFECT included routines for simulating the effects of surface residues on runoff and soil evaporation; the decomposition of surface residue was modelled as a simple function of time. The CERES models treat all residues of previous crops as incorporated into soil, and therefore cannot include any effect of surface residues on the soil water balance. CERES does deal with nitrogen, and simulation of the decomposition of fresh residues takes into account the residue C:N ratio and environmental factors of moisture and temperature. The code of these models has been re-engineered into discrete modules, amalgamating features of both CERES and PERFECT, and enhanced to incorporate aspects that are considered necessary for APSIM to be applicable to the farming systems that are of interest to its users.

In describing the processes that are simulated, the following conventions are used: state variables are denoted by bold lower-case and parameters are indicated by italic lower-case. The APSIM modules are coded in FORTRAN using long, descriptive names; where appropriate, these are used here also.

APSIM SOILWAT v.1

The subroutine structure of the water balance module, SOILWAT, is depicted in Fig. 1, which shows the processes that are considered in the model. It is a cascading layer model and owes much to its precursor in CERES. Code adopted from PERFECT includes: (i) the effects of surface residues and crop

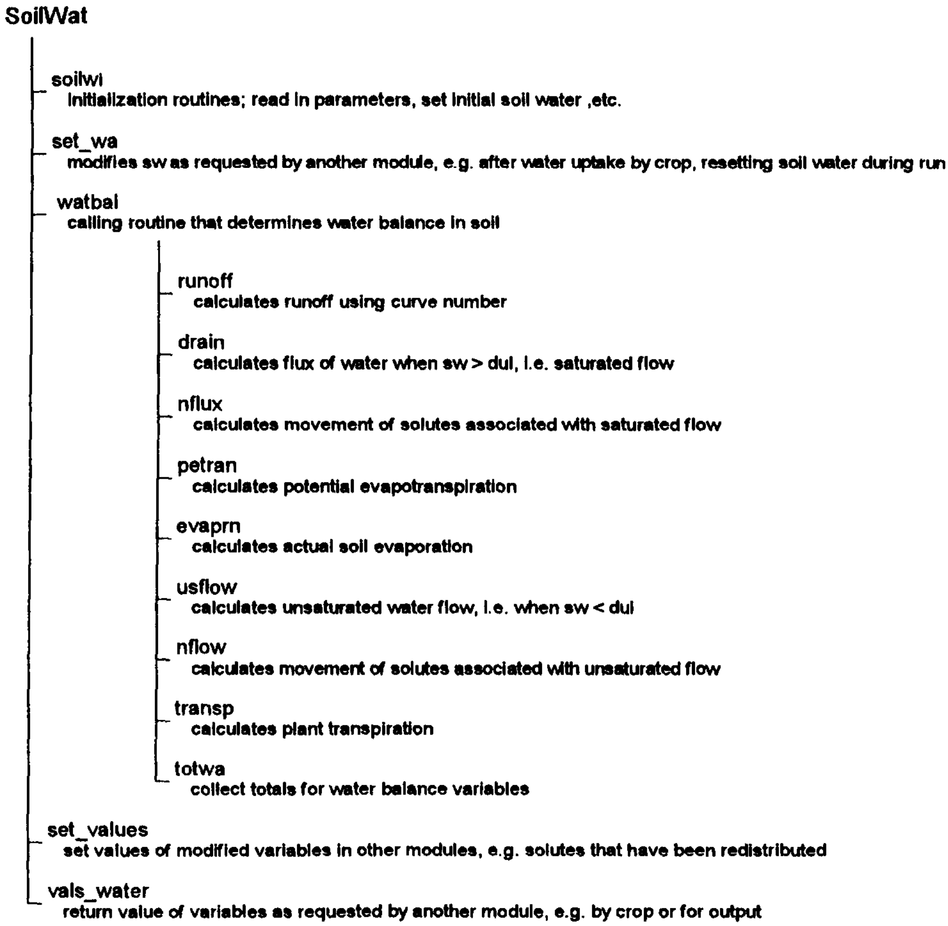

Fig. 1. Simplified subroutine structure of the SOILWAT module to show the processes considered. Note that, in APSIM, routines to determine water use by a crop are part of the crop modules.

cover on modifying runoff and reducing potential soil evaporation; (ii) small rainfall events are lost as first stage evaporation rather than by the slower process of second stage evaporation, and (iii) specification of the second stage evaporation coefficient (*cona*) as an input parameter, providing more flexibility for describing differences in long-term soil drying due to soil texture and environmental effects. The water characteristics of the soil are specified in terms of the lower limit (**ll15**), drained upper limit (**dul**) and saturated (**sat**) volumetric water contents. Other inputs required to specify the behaviour of water in the soil are listed in Appendix 1. It is notable that redistribution of solutes, such as nitrate N and urea N, is carried out in this module. The module is interfaced with the RESIDUE and crop modules so that simulation of the soil water balance responds to change in the status of surface residues and crop cover (via tillage, decomposition, and crop growth).

Enhancements beyond CERES and PERFECT include the specification of *swcon* for each layer, being the proportion of soil water above **dul** that drains in one day, and isolation from the code of the coefficients determining diffusivity as a function of soil water (used in calculating unsaturated flow). On fine textured soils it has been found that the diffusivity coefficients 'hard-wired' into CERES cause too much water to move upwards into the top soil layer, while earlier work (Dimes, 1996) had shown that too little water was moved in a sandy textured soil. Choice of coefficients more appropriate for soil type (Reichardt *et al.*, 1972) was found to improve model performance. Unsaturated flow is permitted to move water between adjacent soil layers until some nominated gradient in soil water content is achieved, thereby accounting for the effect of gravity on the fully drained soil water profile.

APSIM SOILN v.1

All models of nitrogen turnover in soil attempt to capture, to varying degrees, our knowledge of the processes (physical, biological, and physico-chemical) involved, and thus many of them share common features. They differ in the complexity with which they deal with these processes. Added complexity (more mechanistic models) generally results in more information being needed to specify the model, but more complicated models do not necessarily result in improved predictions of observed behaviour (de Willigen, 1991).

Decisions on what degree of complexity should be incorporated into the APSIM SOILN module were largely based on experiences with CERES-Maize and derivatives from it. Although certain soil and crop management effects on the nitrogen supply to a crop could be simulated (e.g. Keating *et al.*, 1991), there were limitations. A single soil organic matter pool, for example, cannot deal realistically with situations where fresh leguminous residues contribute nitrogen to the soil system (Dimes, 1996). Furthermore, treating all the soil organic matter as being equally susceptible to mineralisation (which is the case with CERES) results in unrealistic rates of mineralisation in the subsurface soil layers. This latter aspect, together with the lack of a full carbon balance, made use of CERES for long-term simulations of soil organic matter content inappropriate.

The subroutine structure of SOILN is given in Fig. 2, whilst the transformations occurring to the soil organic matter pools in each layer are shown diagramatically in Fig. 3. The major difference from the CERES model is that the soil organic matter is divided into two pools (**biom** and **hum**), the **biom** pool notionally representing the more labile, soil microbial biomass and microbial products, whilst **hum** comprises the rest of the soil organic matter.

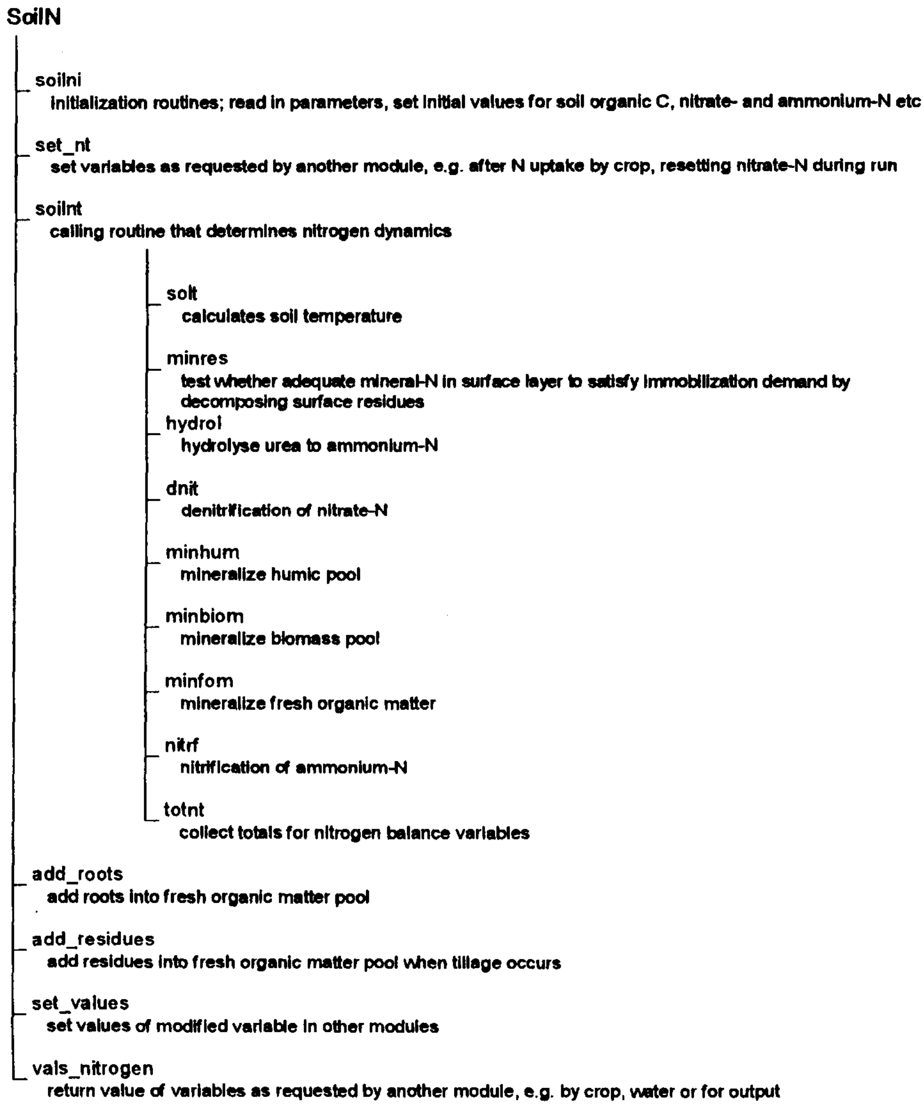

Fig. 2. Simplified subroutine structure of the SOILN module to show the processes considered. Note that routines to determine nitrogen uptake by the crop are part of the crop modules.

The flows between the different pools are calculated in terms of carbon, the corresponding nitrogen flows depending on the C:N ratio of the receiving pool. A constant C:N is assumed for **biom**; C:N for **hum** is derived from the C:N ratio of the soil which is an input.

Decomposition of **biom** and **hum** pools are calculated as first-order processes with the rate constants being modified by factors involving the soil temperature and moisture in the layer. The fresh organic matter pool (**fom**) is treated as in CERES-Maize (Jones and Kiniry, 1986), and its rate of decomposition also depends on a C:N ratio factor. Mineralisation or immobilisation of mineral N is determined as the balance between the release of nitrogen during decomposition and immobilisation during microbial synthesis and humification. An inadequate supply of mineral N to satisfy the immobilisation demand results in a slowing of the decomposition. Both ammonium N and nitrate N are available for immobilisation, though ammonium N is used preferentially.

Decomposition of any organic matter pool results in evolution of carbon dioxide to the atmosphere and transfers of carbon to the **biom** and **hum** pools. The flows are defined in terms of efficiency coefficients, representing the proportion of carbon retained in the system, and the fraction of the retained carbon that is synthesised into the **biom** pool (see Table 1 for parameter definitions and values). When **biom** decomposes there is an internal cycling of carbon (microbes feeding on microbial products).

The reduction of the rate of decomposition of soil organic matter in the subsoil is accomplished by assuming that some of the **hum** pool is not subject to decomposition. In some models, for example CENTURY (Parton *et al.*, 1988), a third soil organic matter pool ('passive') is included which turns over more slowly than the 'active' and 'slow' pools. We choose to achieve much the same outcome, but by a different approach. At initialisation, the proportion of soil carbon in each layer that is inert (finert) is specified and the amount of **inert_C** calculated. The decomposition rate of the **hum** pool then becomes

$$\text{decomp\_C\_hum} = rdhum^{*}\text{mf}\ ^{*}\text{tfac}^{*}(\mathbf{hum} - \mathbf{inert\_C})$$

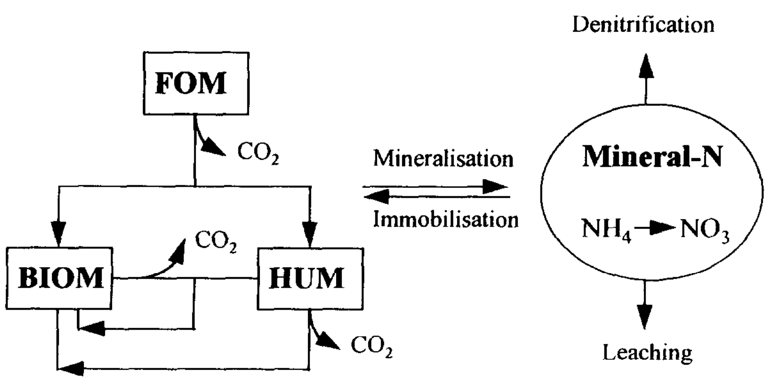

Fig. 3. Schematic representation of the processes affecting soil organic matter and nitrogen transformations in a soil layer.

TABLE 1
Model Parameters Determining the Flows of Carbon during the Decomposition of the Soil Organic Matter Pools and Surface Residues

Parameter	*Value*	*Definition*
mcn	8.0	C:N ratio of **biom** pool
ef_fom	0.4	Efficiency of carbon retention when **fom** decomposes
fr_fom_biom	0.9	Proportion of retained carbon from **fom** synthesised into **biom**
ef_biom	0.4	Efficiency of carbon retention when **biom** decomposes
fr_biom_biom	0.6	Proportion of retained carbon from **biom** resynthesised into **biom**
ef_hum	0.4	Efficiency of carbon retention when **hum** decomposes
ef_res	0.4	Efficiency of carbon retention when residues decompose
fr_res_biom	0.9	Proportion of retained carbon from residues synthesised into **biom**
rdbiom	0.0081 day^{-1}	decomposition rate for **biom**
rdhum	0.00015 day^{-1}	decomposition rate for **hum**

where *rdhum* is the rate coefficient (day^{-1}), and mf and tfac are the factors determining the effects of moisture and temperature. Thus **inert_C** is effectively the organic carbon content that would result from a long period of decomposition without any input of fresh organic matter. It is conceptually similar to the equilibrium value (N_e) in the equation of Bartholomew and Kirkham (1960):

$$N_t = N_e + (N_0 - N_e)exp(-kt)$$

where the equilibrium value represents the steady-state situation that would result from a system with a constant annual accretion of organic matter.

The addition of the **biom** pool results not only in a need for numerous extra coefficients to specify the model (Table 1) but also a requirement to initialise this pool size in each layer. We choose to do this by specifying the proportion of the soil carbon that is present as **biom** (fbiom); it is convenient that fbiom be defined in terms of the **hum** carbon that is subject to decomposition, so that

$$\text{fbiom} = \mathbf{biom/(hum - inert\_C)}$$

Data exist for the proportion of the total soil carbon that is present as microbial biomass in wheat–fallow systems (Jenkinson, 1990; Amato and Ladd, 1994) and in other systems (Anderson and Domsch, 1989), though only for surface soils. Our supposition is that the proportion is substantially lower in subsurface layers, where there are smaller inputs of fresh residues to act as substrate for the soil microbial population. For the schema shown in Fig. 3, it can be shown that, in the absence of **fom**, a steady state will exist (fbiom unchanging through time) when the relative rates of decomposition of **biom** and **hum** are related to fbiom as follows:

$$rdbiom/rdhum = \{1+ef\_hum/\mathrm{fbiom}\}/\{1-ef\_biom^*(fr\_biom-\mathrm{fbiom}^*(1-fr\_biom))\}$$

This expression is helpful for selecting rates of decomposition of the **biom** and **hum** pools which will prevent the model from creating or decomposing unrealistic amounts of microbial biomass, a problem encountered by Dimes (1996) when using a rate coefficient for the **biom** pool derived experimentally from an incubation study. The values of *rdbiom* and *rdhum* in Table 1 are commensurate with a steady-state value for fbiom of 0.01. Because of additions of roots and crop residues, fbiom in the near surface layers of soil will normally be higher than this steady-state value.

APSIM RESIDUE v.1

The surface residue module is a simplistic representation of the system (Fig. 4) with much of the tillage incorporation and cover relationships retained from PERFECT, but a more mechanistic basis for the decomposition of surface residue decomposition is required to maintain the carbon and nitrogen balances. The decomposition algorithm draws on the work of Dimes (1996) but differs from this work by making the moisture term for decomposition a function of cumulative potential soil evaporation rather than the water content of the surface soil. To link decomposition of surface residues to soil water content required data for the immediate surface layer (0–2 cm), which cannot be simulated satisfactorily with SOILWAT. The approach adopted is similar to that used by McCown and Wall (1989) for simulating the decline in quality of forage legumes in tropical Australia.

All above-ground material is considered as a single pool which can be burnt, incorporated into soil as **fom**, or decomposed. Upon decomposition, the products are CO_2, and **biom** and **hum** in the topmost soil layer (see Table 1 for parameters determining the flows of carbon from the surface residues to the soil). Mineral N in the topmost soil layer is allowed to meet any immobilisation demand; if mineral N is inadequate, decomposition of residues is restricted. The temperature constraint on the rate of decomposition is defined in terms of the average daily temperature and the moisture constraint in terms of the cumulative potential soil evaporation since the last rainfall or irrigation event, the moisture factor declining linearly with cumulative evaporation.

The rate of decomposition is also sensitive to the amount of residue on the soil surface. A 'contact' factor accounts for the opposing effects of mulch separation from the soil surface and a modified moisture environment in the mulch layer as the amount of surface material increases. The function currently used is based on very limited data (Dimes, 1996).

Tillage transfers a proportion (*f_incorp*) of the residue to the soil **fom** and distributes it to the nominated depth. Within a typical APSIM simulation, tillage operations would normally be specified in terms of the implement used and associated values of *f_incorp* and depth of incorporation obtained from a lookup table.

The surface residue pool is characterised in terms of its C:N ratio and specific area; when material is added, for example when a crop is harvested, new values are calculated as weighted averages for the whole of the residues. The specific area is used to calculate the cover due to the residues, which is used in the SOILWAT module to modify the runoff curve number, and thus runoff and also evaporation.

Sources of data for evaluating model performance

Two sets of experimental data, which provide a contrast in soil type and climate, are used here for testing the performance of the model in predicting changes in soil water and nitrate N. These data are from replicated experiments and the observed data used for comparison with simulated values are treatment means.

The first data set comes from the Fertility Restoration Experiment at Warra, Queensland (Dalal *et al.*, 1996). The soil at this site is a vertisol but

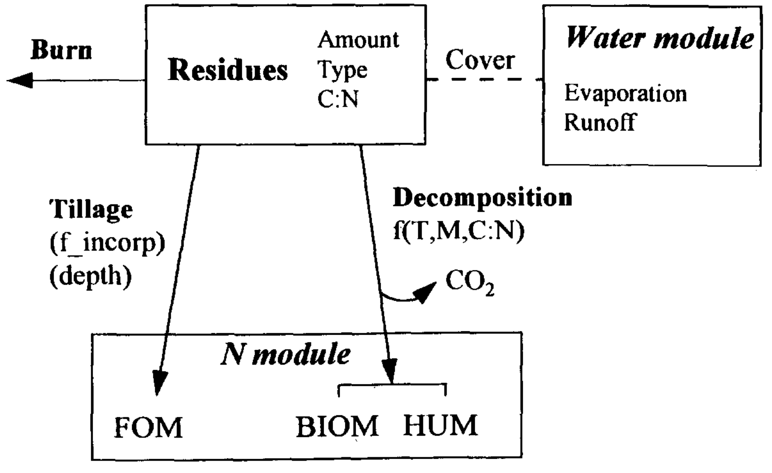

Fig. 4. Schematic representation of the processes dealt with in the RESIDUE module.

many years of cropping prior to the commencement of the experiment had depleted the soil of much of its original fertility. For the present purposes, only a subset of the treatments is considered, these being the continuous wheat plots that compare conventional and zero tillage with three rates of applied nitrogen (0, 25, and 75 kg N ha^{-1}). Wheat was grown in 1987 and each subsequent season with the exception of 1991 (when rainfall was inadequate to provide a planting opportunity). All crop residues were retained. Soil sampling for determination of soil water content and nitrate N in the profile was carried out twice per year, prior to planting (in May) and post-harvest (October/November). Soil cores are sectioned into the depth intervals 0–10 cm, 10–20, 20–30, and then in 30 cm increments to 1.5 m.

Simulation of the experiment was carried out by running the model from November 1987, after the crop harvest, to the preplant sampling in May 1994. Each year the soil water and nitrate N were reinitialised with measured data from the post-harvest samplings, when above-ground residues and roots were also added. Data are available for the actual yields of crop residues and their N content, but an assumption had to be made for estimates of roots. We assume that 20% of total crop carbon was in roots with a C:N ratio of 40. The performance of the model was tested by comparing observed and predicted water and nitrate N data at the next pre-plant sampling. When no crop was grown, as in 1991, the comparison was continued through the long fallow.

The second source of data is from experiments at Katherine, Northern Territory (Dimes, 1996), where changes in soil water and nitrate were measured during fallows on both a Fenton clay loam and a Venn sandy loam (alfisols) after preceding legume ley pastures had been chemically killed. These experiments were for a single season 1985–1986, but soil water was measured on fourteen occasions and nitrate N four times. When soil was sampled for nitrate N analysis, soil water was obtained from gravimetric moisture determination but on other occasions soil water estimates were obtained from neutron moisture meter measurements. Simulation of these experiments was carried out by initialising the model at the beginning of the experimental period using measured data for soil water, nitrate N, and residues on the soil surface (amount and C:N ratio). The amount of root residues following the forage legume pasture was based on a root:shoot ratio of 2:1. Predictions of soil water and nitrate N were compared with the observed data.

These data sets do not include any measurement of runoff, and therefore provide no opportunity to test the predictive capability of the model with regard to this important component of the water balance. We address this using a third data source from a contour bay catchment study at Greenmount, Queensland (Freebairn and Wockner, 1986; Silburn and Freebairn, 1992). Rainfall, runoff, and soil moisture were measured from unreplicated catchments of about 1 ha under winter cereal–summer fallow systems. Both zero tilled (six fallows) and conventionally tilled (eight fallows) are represented in this data set. The soil at this site is also a vertisol. Soil water was measured as the average of gravimetric determinations to 1.5 m at nine locations in each catchment. To simulate this experiment the model was initialised at the soil sampling after harvest of the crop each year and run until the sampling prior to planting the next crop. Inputs were soil water profiles and residues from the previous crop, which were assumed to have a C:N ratio of 80. In some fallows there were several samplings for soil water. We use the period between sampling occasions as the time base for comparing predicted runoff with the measured data.

Choice of parameters and initialisation of state variables

Considerable experience has been gained from earlier efforts to model aspects of water and crop growth on the cracking clay soils of the Darling Downs (for example Littleboy *et al.* 1992; Probert *et al.*, 1995) and for changes in water and nitrogen at the Katherine sites (Dimes, 1996). The models used in these studies provide estimates for most of the parameters required here for the simulation of soil water.

For the Warra site, which has not previously been modelled, estimates for **ll15** and **dul** were derived from the observed soil water data at the site (not necessarily for the wheat plots) using the driest and wettest soil water contents measured during the experiment; **sat** was estimated as total porosity less 0.05 for entrapped air when the soil was fully wet.

For nitrogen, specification of model parameters and initialisation of the state variables requires that several assumptions be made, the validity of which has to be judged from the performance of the model. Firstly the amount of soil carbon that is considered to be inert. It is presumed that most of the carbon in the deep subsoil is not susceptible to decomposition and that similar amounts of **inert_C** are present in the upper layers of soil. Taking the Warra profile as an example (Appendix 1), it has been assumed that 0.4% organic carbon is inert (total organic C in the deepest, 1.2–1.5 m, layer is 0.43%), from which the fraction of inert C in all layers is calculated. For vertisols where the concentration of organic C decreases smoothly with depth, this is a reasonably straightforward approach, but it is more subjective for the alfisols from Katherine.

Typically some 2% of the total organic C in the surface soil is measured as microbial biomass C in cereal systems (Jenkinson, 1990; Amato and Ladd, 1994). In subsoils, the proportion is likely to be considerably less than this because there is less substrate (roots and incorporated crop residues) to support the microbial population. As discussed above, in the absence of **fom**, a steady-state situation can be expected where the **biom** pool is sustained solely by the soil organic matter, and the equation given provides a means of choosing fbiom for the deeper soil layers and the relative rates of decomposition of **biom** and **hum** so that the model will stay within bounds. For long-term experiments, the sensibleness of the initial estimates for fbiom can be judged from how the **biom** pool is predicted to change through time. Under a continuous wheat-fallow system, it would be expected that changes in **biom** would be cyclical within a year, but without any long-term trend for build-up or run-down of this pool. However, such data sets are not well suited for evaluating how large the **biom** pool should be; provided **biom** remains near constant through time, the model will be insensitive to its magnitude. The Katherine experiments relate to situations where legumes had been grown previously. Here we assume that fbiom in the uppermost soil layers would initially be higher than the following cereal crops, and some of the net mineralisation measured will result from a decrease in the **biom** pool during the ensuing fallow.

Values for the parameters defining flows of carbon and nitrogen between the various pools (Table 1) are estimates based on what has been used by others in similar models (e.g. Johnsson *et al.*, 1987; Parton *et al.*, 1988; Bradbury *et al.*, 1993). A value is required for the rate of decomposition of the **hum** pool (*rdhum*). In CERES, where all the soil organic matter is assumed to decompose at the same rate, the value used is 8.3×10^{-5} day^{-1}. Here we consider part of the soil organic matter to be inert; so, to mineralize the same amount of N, a higher value for the rate of decomposition will be needed. We have found that setting *rdhum* to 1.5×10^{-4} day^{-1} gives reasonable prediction of changes in soil nitrate N across a range of data sets that we have studied. This value was not tuned specifically to the data sets that are reported here.

Statistical comparison of observed and predicted data

No single statistic gives an adequate overall measure of the goodness of fit between observed and predicted values. Testing whether the intercept and slope of the fitted linear regression between observed and predicted values differ significantly from zero and unity, respectively, is a rigorous test, but is sensitive to outliers that can have undue influence on the fitted line. We choose to present the coefficient of determination (R^2) as a measure of the association between observed and predicted values and the root mean squared deviation (RMSD) as an indicator of deviations from the expected 1:1 line; the difference between the RMSD and the residual standard error (RSE) about the fitted line is an indicator of departure from the expected 1:1 relation.

RESULTS

The simulated time course for changes in soil water and nitrate N for one of the treatments of the Warra Experiment is illustrated in Figs 5 and 6. These figures indicate how the soil water and nitrate N profiles were reinitialized at the beginning of each fallow, and the agreement between simulated and observed data at the end of the fallows (and during the long fallow of 1990–1992). In general there is reasonably good agreement, and this is reflected not only in the total water and nitrate N but also in their distribution in the profile as shown for the individual sampling occasions. In some fallows (e.g. 1987–1988 and 1993–1994) there were increases in water content throughout the whole profile whilst in 1992–1993 there was little change in water content of the deeper layers; in both cases the simulated results give a good prediction of the observations. Similarly there is close correspondence in the soil nitrate profiles.

The ability of the model to simulate soil water and nitrate across the range of treatments from the Warra Experiment (2 tillage managements × 3 N rates) is shown in Figs 7 and 8 as plots of observed vs. predicted, where all occasions on which comparisons can be made are included. The statistics of these plots are summarised in Table 2.

For soil water (Fig. 7), the total water in the profile and the volumetric water content in the individual soil layers lie close to the 1:1 lines, with no obvious effects of treatments on the closeness of fit. For soil nitrate N (Fig. 8) the closeness of fit is best at the lowest rate of fertilizer application; the nitrate N concentrations in the individual soil layers for the 75 kg ha^{-1} rate show considerably greater spread about the 1:1 line though there is no indication of bias. A contributing factor to this lack of fit is the markedly greater variance (between replicates) in the observed soil nitrate data for the highest rate of fertilizer application; the pooled standard error of treatment means for nitrate N concentration in the top three soil layers was 0.78, 1.29, and 4.53 mg kg^{-1} for the three fertiliser treatments. This probably reflects shortcomings in the sampling strategy to recover residual nitrate in the soil from the banded fertilizer, especially in years with low rainfall when uptake of the applied nitrogen was low and little leaching occurred to redistribute it through the soil profile.

The time course of simulated and observed data, together with depth profile plots for volumetric water content and soil nitrate N concentrations on selected days, for the experiments at Katherine are shown in Figs 9 and 10. For both the clay loam and the sandy loam the prediction of soil water closely agrees with the observed data, especially the initial rewetting of the soil profile and the subsequent drying of the soil to 30 cm on the clay loam (day 56) and greater depth in the case of the sandy loam (days 51 and 83).

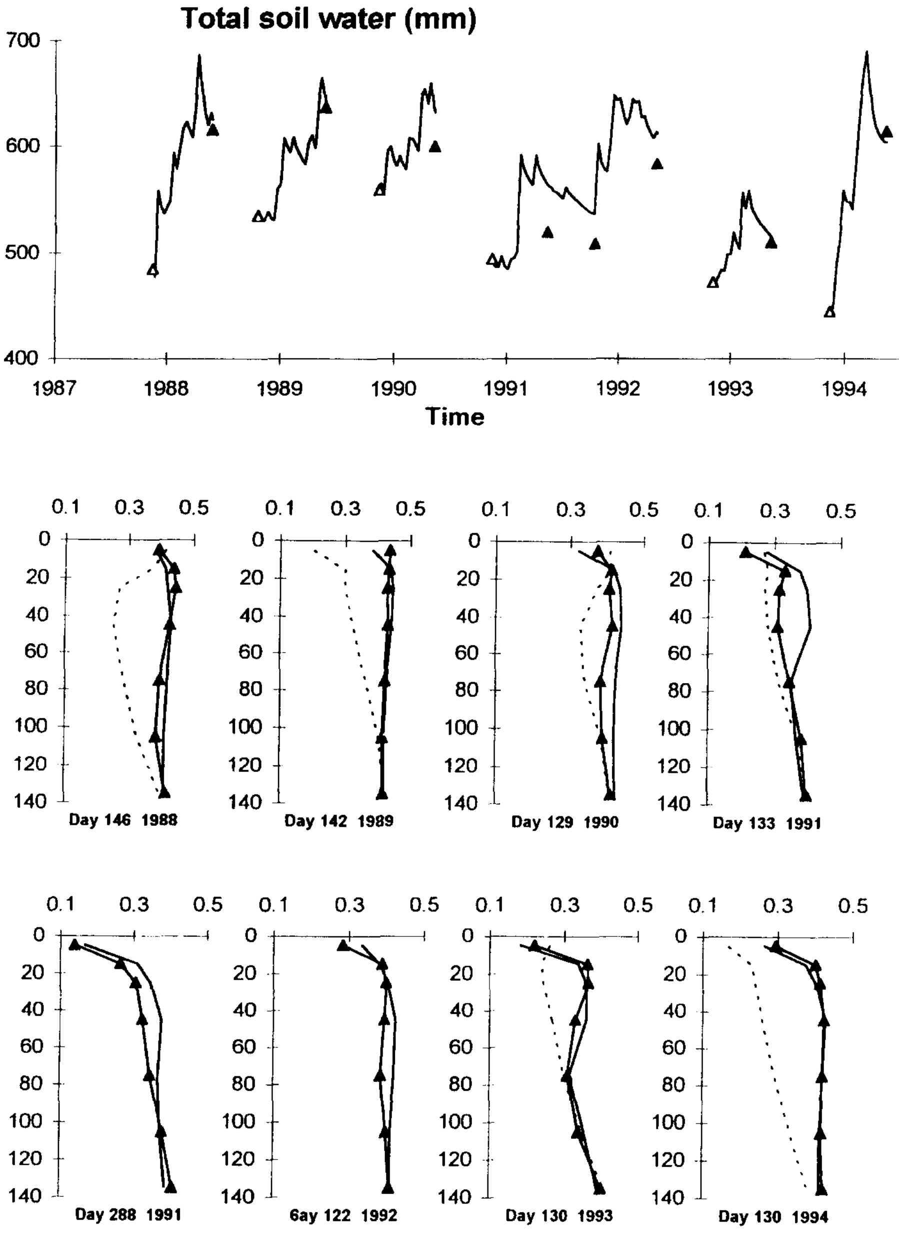

Fig. 5. Comparison of simulated and measured soil water during the fallows for the conventional tillage, zero N treatment at Warra. The main figure shows the simulated total soil water in the 0–150 cm profile as the continuous lines (plotted every 20 days) with observed data as symbols (open symbols denoting the post-harvest data used to reinitialise the model). The small graphs at the bottom of the figure show the simulated (solid lines) and observed (solid lines with symbols) depth profiles for volumetric soil water content on the days indicated; the dashed lines are the observed water profiles at the beginning of each fallow period.

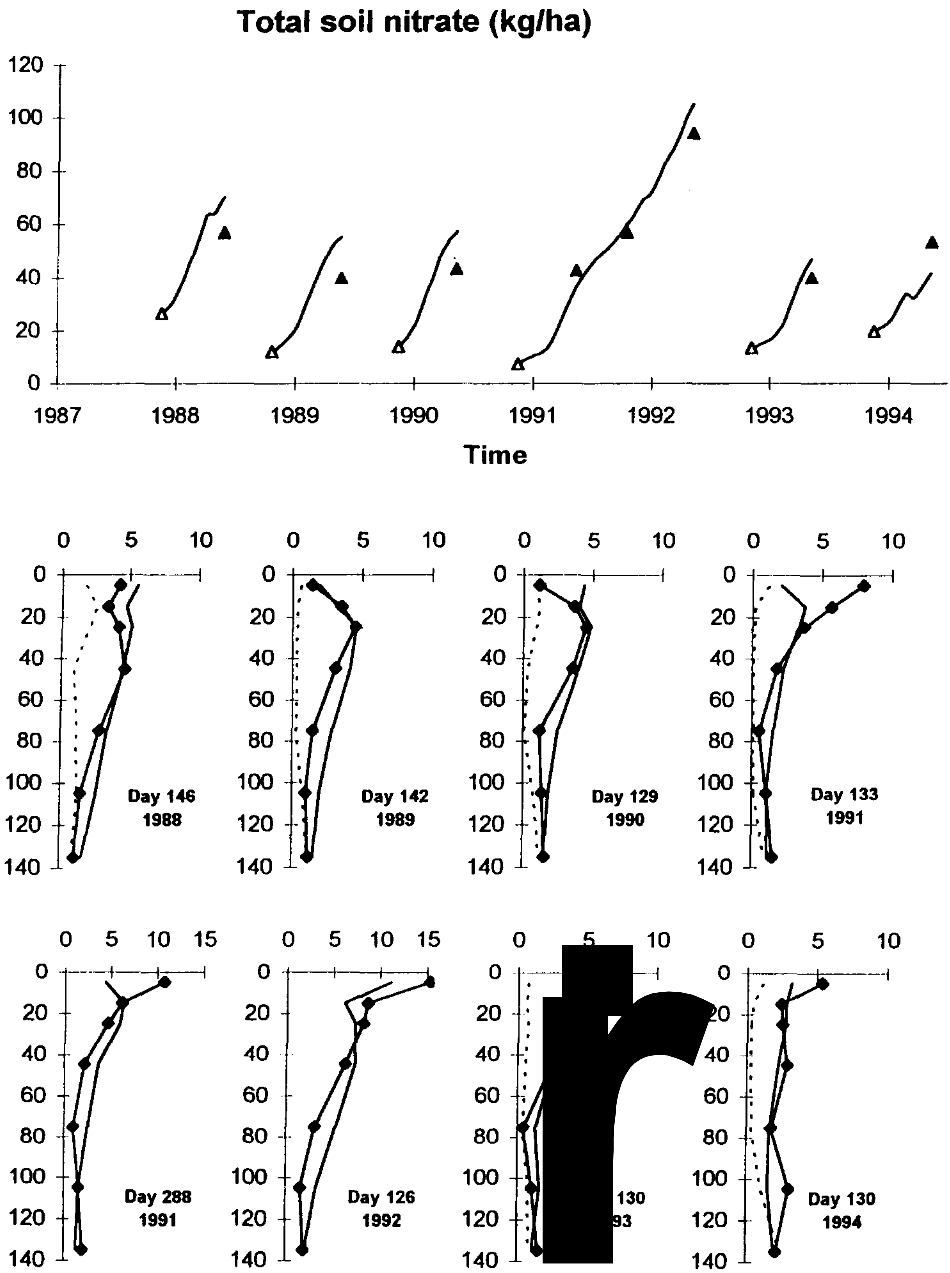

Fig. 6. Comparison of simulated and measured soil nitrate N during the fallows for the conventional tillage, zero N treatment at Warra. The figure is similar to Fig. 5 with the upper part showing the total nitrate N (kg ha^{-1}) in the 0–150 cm profile and the small graphs the depth profiles for nitrate N concentration (mg kg^{-1}).

TABLE 2
Statistics of the Closeness of Fit for the Simulated Soil Water and Nitrate N Data at Warra

Site/treatment[a]		*Variable*[b]	*Number of observations*	R^2	*RSE*	*RMSD*
Warra	Tc	swdep	24	0.76	25.1	29.7
	Tz		24	0.82	18.5	21.5
	all		48	0.79	21.6	25.9
Warra	Tc	sw	168	0.77	0.029	0.031
	Tz		168	0.88	0.020	0.022
	all		336	0.82	0.025	0.027
Warra	N0	total NO_3	16	0.82	9.8	10.9
	N25		16	0.78	11.6	11.0
	N75		16	0.67	25.9	24.5
	all		48	0.80	16.7	16.7
Warra	N0	NO_3 conc	112	0.72	1.12	1.64
	N25		112	0.73	1.21	1.59
	N75		112	0.67	2.74	2.79
	all		336	0.70	1.94	2.08

[a] Treatments denoted as Tc = conventional tillage, Tz = zero tillage; nitrogen treatments as kg N ha^{-1} $year^{-1}$.
[b] Variables are swdep = total soil water (mm) in whole profile, sw = volumetric soil water in individual soil layers, total NO_3 = total soil nitrate (kg ha^{-1}) in whole profile, and NO_3 conc. = nitrate N concentration (mg kg^{-1}) in individual soil layers.
R^2 is the coefficient of determination between predicted and observed; RSE is the residual standard error about the fitted linear regression between predicted and observed values; RMSD is the root mean squared deviation.

Because the experimental soils were kept free of vegetation, the range of total soil water is not very large in these experiments and for much of the period the water content in the subsoil remains near the **dul** of these soils. The build-up of total nitrate N in the soils is predicted accurately, with the exception of the observed value on day 58 for the sandy loam soil (Fig. 10). The observed changes in nitrate N distribution in this soil are difficult to understand. The accumulation of nitrate, especially in the deeper layers between days 30 and 58, occurred when there was very little rainfall to move nitrate down the profile; similarly there seems to have been insufficient rain to remove this deep nitrate from the profile between days 58 and 92.

The comparison of simulated and observed data for the Greenmount experiment is set out in Fig. 11. Soil water, plotted as the plant available water in the 0–150 cm profile for each sampling occasion, has an RMSD of 37.7 mm but with no discernable bias from the 1:1 line. Deviations between observed and predicted are greater than for the other datasets but this is not unexpected since the catchments comprise much larger experimental units than the plots at the other sites. Predicted runoff, cumulative for the periods

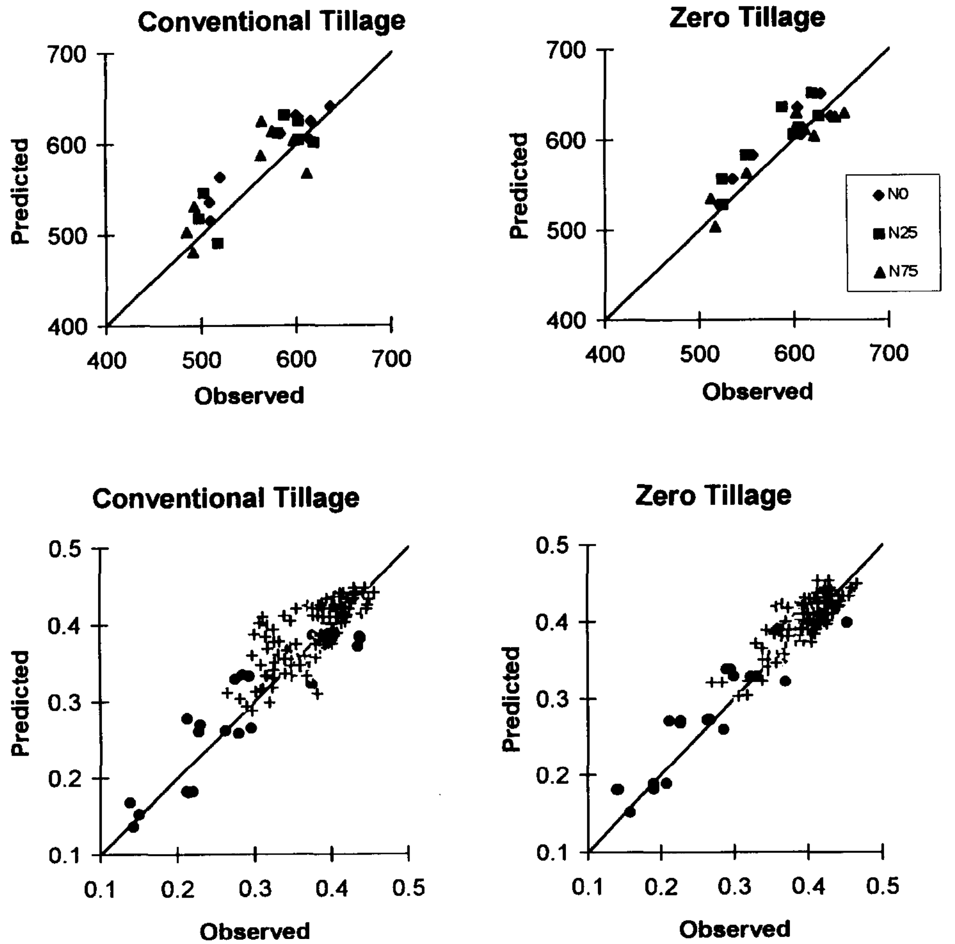

Fig. 7. Observed vs. predicted plots for soil water for six treatments at Warra. The plots at the top of the figure compare the total soil water (mm) in the 0–150 cm profile for conventional and zero tillage. The two lower plots compare the volumetric soil water contents for all of the soil layers, the data for the 0–10 cm layer being distinguished as solid symbols. In each case the 1:1 line is shown.

between soil samplings, agrees closely with the measured data for all but three of the observations. The RMSD of 16.5 mm is greatly inflated by these outliers, all of which overpredicted runoff, and for which we have no satisfactory explanation. All three outliers are for periods following reinitialisation of the model at the commencement of a fallow so could be associated with poor estimates for the initial soil water content. Neither the soil water nor runoff data suggest any difference in model performance between the zero and conventional tillage systems.

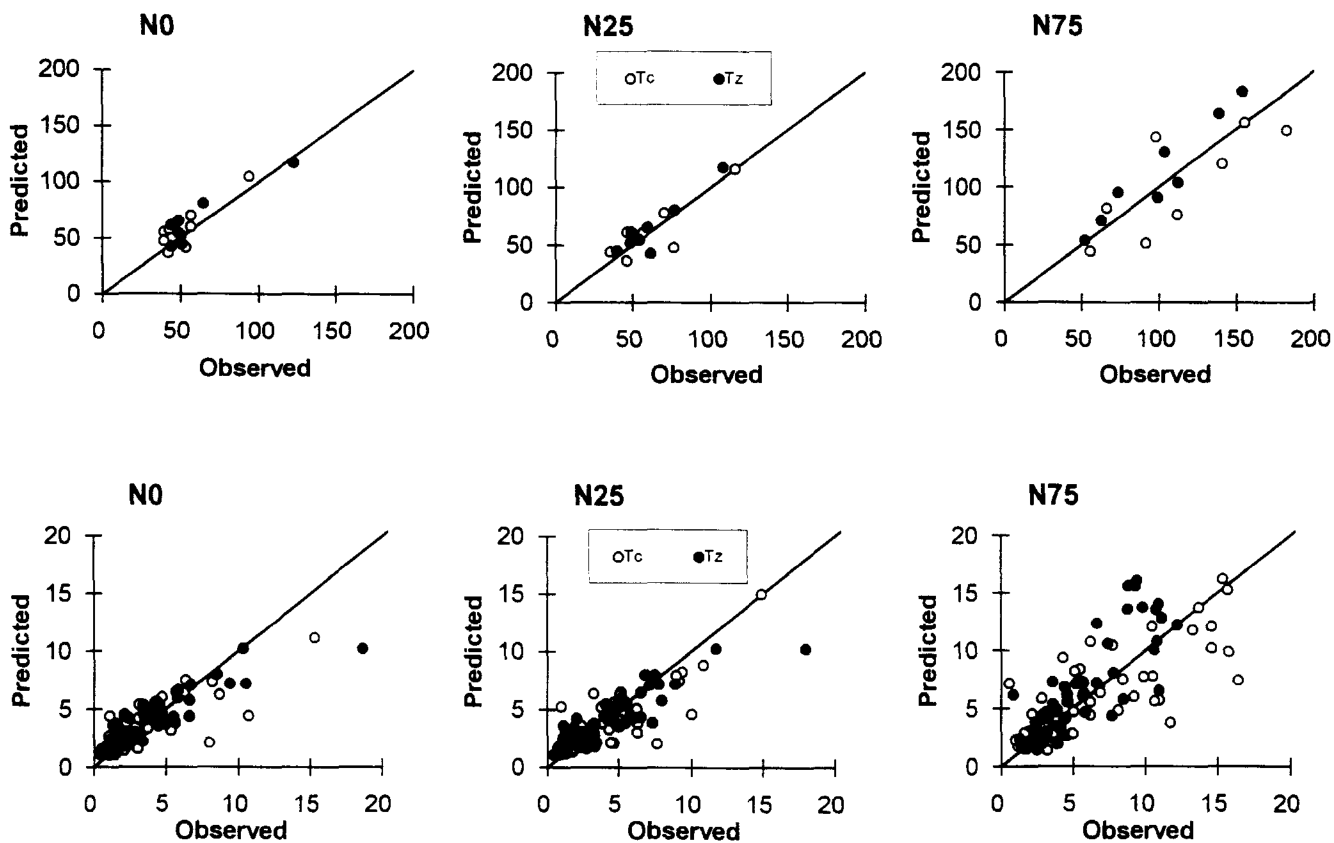

Fig. 8. Observed vs. predicted plots for soil nitrate for six treatments at Warra. The upper plots compare the total nitrate N (kg ha^{-1}) in the 0–150 cm profile for the three rates of nitrogen application; conventional tillage treatments (open symbols) are distinguished from zero tillage (solid symbols). The lower plots compare the nitrate N concentrations (mg kg^{-1}) for all of the soil layers.

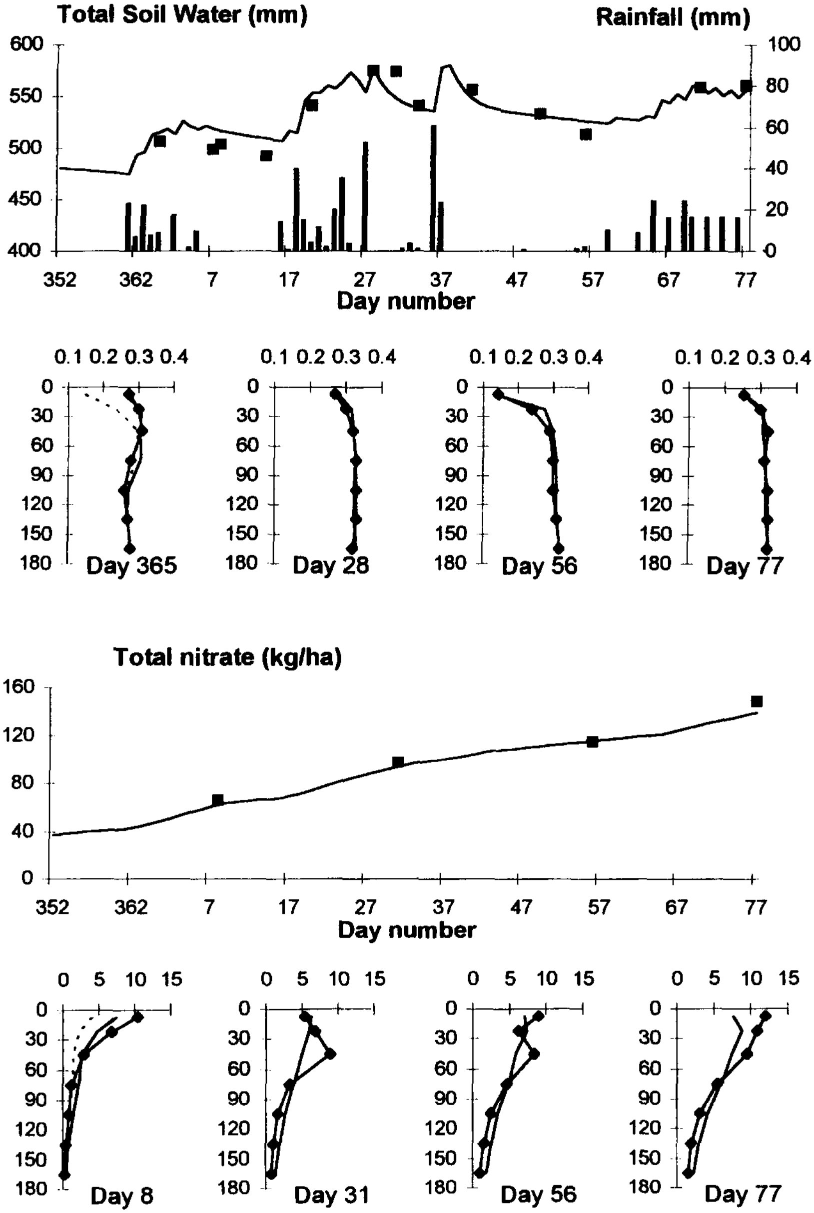

Fig. 9. Comparison of simulated and measured soil water and nitrate N on the Fenton clay loam at Katherine. The upper part of the figure shows the simulated total soil water (mm) in the 0–180 cm profile as the continuous line (plotted every day) with observed data as symbols and daily rainfall and irrigation as vertical bars; the small graphs show the simulated (solid lines) and observed (solid lines with symbols) depth profiles for volumetric soil water content on the days indicated, with the observed water profile at the beginning of the experimental period as the dashed line. The lower part of the figure presents the soil nitrate N in similar fashion, the small plots being the depth profiles for nitrate N concentration in the soil (mg kg^{-1}).

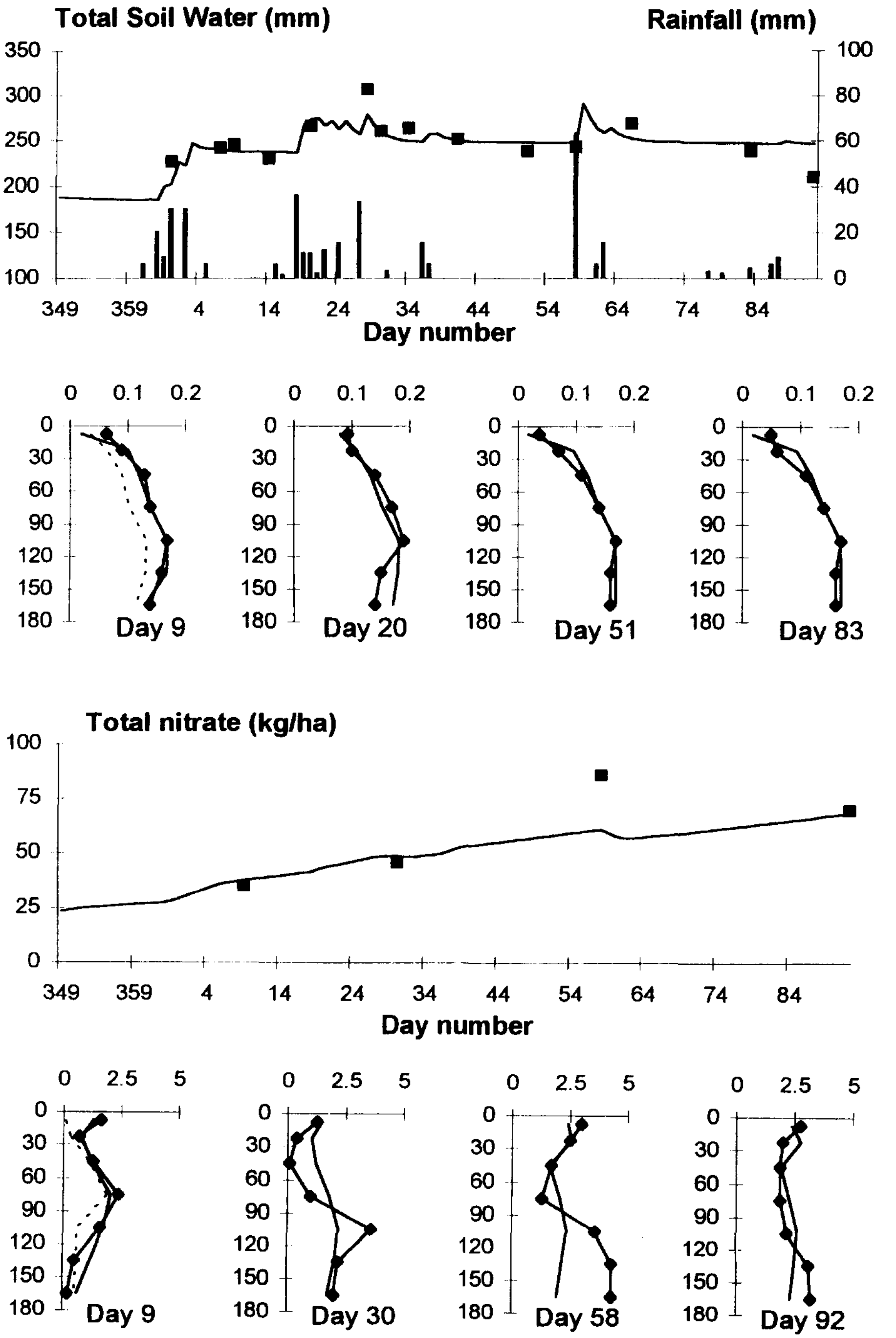

Fig. 10. Comparison of simulated and measured soil water and nitrate N on the Venn sandy loam at Katherine. The style of presentation is identical to that used in Fig. 9.

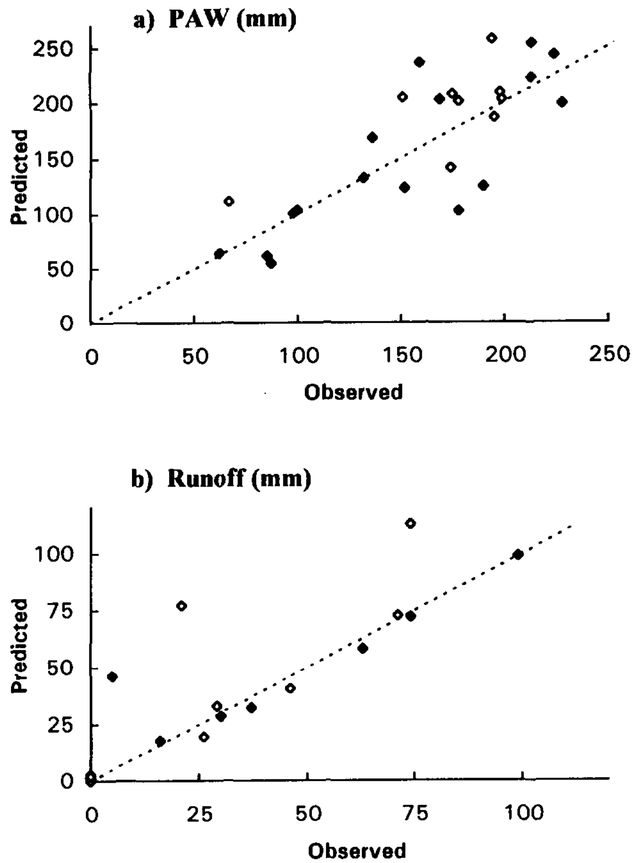

Fig. 11. Comparison of simulated and measured soil water and runoff for the Greenmount experiment. Open symbols denote the zero till treatments; solid symbols are for conventional till; the 1:1 lines are shown.

DISCUSSION

The three APSIM modules described here (viz. SOILWAT, SOILN, and RESIDUE) are part of a suite of modules that can be configured to simulate a diverse range of farming systems. It is anticipated that the APSIM modelling framework will contribute to the analysis of alternative management strategies with respect to both the economics of production and the consequences for the soil resource. To achieve this, it is a prerequisite that the modules are capable of simulating, with an adequate degree of accuracy, the key state variables, which for many dryland farming systems means the dynamics of soil water and nitrogen.

In this paper we have simplified the task of evaluating the performance of these modules by considering fallows only. Whilst this avoids complications due to a crop (and concerns about whether its use of water and uptake of nitrogen are being simulated correctly), there are some undesirable aspects. Notably for the Warra dataset, there are implications for the turnover of soil organic matter. Firstly there can be no carbon inputs due to root death during the growth of the crop, and secondly the soil moisture status will not be correctly simulated during the period when the crop would be growing, which will influence the decomposition of the soil organic pools.

The modelling of soil water during the fallows was a greater challenge than we had anticipated. When modelling crop growth, much of the water removed from the soil is through transpiration, but in a fallow there is greater demand to predict soil evaporation correctly. For the Warra and Katherine data sets, the closeness of fit has to be judged on changes in soil water content and its distribution within the profile, because other components of the soil water balance are not known. This requires the model to correctly simulate the balance between infiltration (and therefore runoff), redistribution in the profile, and subsequent evaporation. More infiltration (smaller value for *cn2*) can be counteracted by more evaporation (larger *cona*); redistribution in the profile is controlled by the coefficients determining the diffusivity. In the absence of experimental data for the runoff and/or drainage components of the water balance, there is no certainty that the parameter values we have used are the correct mix, as different combinations of parameter values could yield similar outcomes for soil water content.

The data from the Greenmount experiment permits a separate evaluation of model performance in terms of its capability to simulate runoff. This showed that generally the agreement with measured data was very satisfactory, though it is unfortunate that three unexplained outliers lessen the claim that the model does adequately predict runoff.

The code for unsaturated water flow invokes soil diffusivity. We have found that for the vertisol at Warra, and on other similar soils (data not presented), better predictions of soil water are obtained with a smaller value for diffusivity than that built into the CERES models. Too high a diffusivity causes rapid upward movement of water; the water content of the topmost soil layer remains aligned with that of the second soil layer so that as the soil dries out the soil water gradient is too small.

The coefficient for second stage evaporation in the CERES models was assumed to be a soil resistance to water loss that was constant for all soils. In PERFECT it was isolated as an input (*cona*), that could be varied with soil type, and this has been retained in the SOILWAT module. However, our experience has been that it is not easy to choose an acceptable value for *cona*. There is theoretical and empirical evidence that *cona* varies with evaporative demand (Boesten and Stroosnijder, 1986), and future revisions of SOILWAT may need to account for this.

The parameters for the SOILN module have not been selected on the basis of tuning them to a particular data set. Rather, we have been guided by previous modelling endeavours and our understanding of the system. The values chosen (Table 1) have been applied to the various experimental data sets and, in terms of predicting changes in nitrate N, model performance is generally good. However, this is not to say that some refinement of the parameter values may not be necessary. Nitrate N in soil is only one aspect of the soil resource. Long-term changes in soil organic matter content is a major issue for sustainable farming systems. Probert *et al.* (1995) provided some evidence that both SOILN and CENTURY predicted the decline in soil organic matter content that occurred in a continuous cereal cropping system with different fertilizer inputs and tillage/residue managements, but the model performance in terms of soil organic matter for other farming systems remains to be evaluated.

There is no doubt that the most difficult part of the SOILN module to verify, or specify for any given situation, is that relating to the notional soil microbial biomass (**biom**). The inclusion of the **biom** pool in the structure of the SOILN module results in it being too complicated to fully evaluate with data from cereal–fallow rotations alone. This pool has been included because of an expectation that it will be needed to cope with (legume) ley–cereal systems. We surmise that in continuous cereal systems, there is little change from year to year in the magnitude of this pool. So provided the model does not predict this pool to be building up or releasing its nitrogen, it is immaterial what the actual size of the pool is. A better understanding of how it varies under different managements will come from studies on systems with other crops, including legumes and pastures, and should lead to guidelines on how it can be initialised.

With the caveats outlined above, the model predicts the observed soil water and nitrate N dynamics during the fallows of the Warra experiment reasonably well, and also provides a good fit for the data sets from Katherine, which are for very different soils and climatic conditions. It should be stressed that the model parameters defining the rates of decomposition of the various soil pools and the flows of carbon and nitrogen between pools are identical for all data sets. Therefore it would seem that the APSIM modules are robust in the sense that they will be widely applicable. When comparing the performance of several models for soil nitrogen, de Willigen (1991) concluded 'that the simulation of the above ground processes was less problematic than that of the below ground processes'. However, our experience is that these APSIM modules do capture the dynamics of nitrate N in soil sufficiently well to be used along with other modules in the simulation of diverse farming systems.

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APPENDIX 1

TABLE A1

Inputs required to specify the SOILWAT and SOILN modules

a) Soil properties and initial values by layers

layer	1	2	3	4	5	6	7	Layer number
dlayer	100	100	100	300	300	300	300	Layer depth (mm)
ll15	0.23	0.24	0.24	0.25	0.26	0.27	0.28	Lower limit soil water content (volumetric)
air_dry	0.10	0.24	0.24	0.25	0.26	0.27	0.28	Water content to which soil can dry by evaporation
dul	0.45	0.46	0.46	0.46	0.44	0.43	0.43	Drained upper limit (volumetric)
sat	0.50	0.51	0.51	0.51	0.49	0.48	0.48	Saturated water content (volumetric)
sw	0.414	0.375	0.270	0.253	0.286	0.326	0.396	Initial soil water content (volumetric)
bd	1.30	1.30	1.29	1.31	1.35	1.36	1.36	Bulk density (g dry soil per cm^3 moist soil)
oc	1.03	0.86	0.77	0.65	0.54	0.48	0.43	Organic carbon (%)
ph	8.2	8.5	8.6	8.6	7.4	5.5	5.0	Soil pH
nh4	1.3	1.0	1.0	0.8	0.8	0.5	0.5	Initial ammonium N (mg kg^{-1})
no3	1.75	2.58	2.12	0.99	1.20	1.28	0.94	Initial nitrate N (mg kg^{-1})
finert	0.39	0.47	0.52	0.62	0.74	0.83	0.93	Proportion of initial organic C assumed to be inert
fbiom	0.035	0.02	0.015	0.01	0.01	0.01	0.01	Initial **biom** as proportion of non-inert C
swcon	0.2	0.2	0.2	0.2	0.2	0.2	0.2	Proportion of water above dul that drains each day

b) Soil water parameters

u	6	Stage 1 soil evaporation coefficient (mm)
cona	5	Coefficient for stage 2 soil evaporation (mm $day^{-0.5}$)
cn2	80	Runoff curve number
cn_red	20	Maximum reduction in cn2 due to presence of surface residues
cn_cv	80	Percentage residue cover at which maximum reduction in cn2 occurs
salb	0.13	Bare soil albedo
diffus_const	40	Coefficient defining diffusivity
diffus_slope	16	Coefficient defining diffusivity

Table A1—*contd*

c) Soil nitrogen parameters		
amp	15.0	Temperature amplitude (°C) = difference between highest and lowest mean monthly air temperatures
tav	20.0	Mean annual air temperature (°C)
dmod	1.0	Factor to adjust rate of mineralisation where organic matter is chemically or physically protected
soil_cn	14.5	C:N ratio of soil
root_wt	2040	Initial root residues (kg ha^{-1})
root_cnr	40	C:N ratio of root residues
residue_wt	5000	Initial surface residues (kg ha^{-1})
residue_cnr	100	C:N ratio of surface residues
residue_type	wheat	Type of surface residues, specific area obtained from lookup table in RESIDUE module
pot_decomp_rate	0.1	Potential decomposition rate of surface residues under optimal conditions (day^{-1})

Values are for the Warra Experimental Site with initial soil water, nitrate N, roots, and surface residue data for the conventional tillage, zero N treatment following the 1987 crop.